The Studies of Geometrical Microstructure of Tetragonal Co^{2+}-V_O Centers in $KNbO_3$ and $KTaO_3$ Crystals from EPR Data

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From the perturbation formulas for the EPR g factors $g_{\|}$ and $g_{\perp}$ of a $3d^7$ ion in tetragonal octahedral crystal field based on a cluster approach, the geometrical microstructures of tetragonal Co^{2+}-V_O centers in $KNbO_3$ and $KTaO_3$ crystals are obtained by fitting the calculated $g_{\|}$ and $g_{\perp}$ to the observed values. It is found that the Co^{2+} ion in Co^{2+}-V_O centers is displaced away from the oxygen vacancy V_O by 0.3 Å in $KNbO_3$ and by 0.29 Å in $KTaO_3$. These results are comparable with those of Fe^{3+}-V_O centers in ABO_3 perovskite-type crystals obtained from both the shell-model simulations and the embedded-cluster calculations, and from theoretical studies of EPR data. The experimental values of $g_{\|}$ and $g_{\perp}$ for the tetragonal Co^{2+}-V_O centers in both crystals are also explained reasonably.

Key words: Electron Paramagnetic Resonance (EPR); Crystal- and Ligand-Field Theory; Defect Structure; Co^{2+}; $KNbO_3$; $KTaO_3$.